Coupling of Parallelized DEGAS 2 and UEDGE Codes

D. P. Stotler, C. F. F. Karney
Princeton Plasma Physics Laboratory
Princeton University

M. E. Rensink, T. D. Rognlien
Lawrence Livermore National Laboratory
Livermore, CA

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INTRODUCTION

- Massively parallel computers more widely available,
- Monte Carlo algorithm scales well with $N_{\rm proc}$,
- $\Rightarrow$ Realism of Monte Carlo codes obtainable with short runs.
- Coupled UEDGE-DEGAS 2 follows success of B2-EIRENE,
- $\Rightarrow$ practical tool for analyzing experiments
  & predicting conditions in future devices,
  - Need techniques for minimizing impact of MC noise.

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DEGAS 2 - EIRENE BENCHMARK

- Use UEDGE slab single-null geometry & plasma,
- Same atomic and surface physics in DEGAS 2 & EIRENE,
- Include recombination,
  - Plasma $T_{e,i} \sim 1$ eV
    $\Rightarrow$ highlights numerical differences.
  - Identify, then eliminate or minimize.
- Each run uses 80,000 flights,
  - $\Rightarrow \sim 1\%$ statitistical error,
- Codes agree to within 5%,

$$\epsilon_{\mathrm{rel}} = \frac{\mu_K^{\mathrm{D}} - \mu_{K'}^{\mathrm{E}}}{\max\left(\sqrt{(s_K^{\mathrm{D}})^2 + (s_{K'}^{\mathrm{E}})^2}, \sigma_{\mathrm{min}} \frac{\mu_K^{\mathrm{D}} + \mu_{K'}^{\mathrm{E}}}{2}\right)},$$

  - Where μ_K = mean for K flights,
  - $s_K = \sigma_{\mathrm{rsd}} \mu_K =$ standard error.
  - Apply to zones with $\sigma_{\mathrm{rsd}} < 20\%$ (Central Limit Theorem),
  - $\sigma_{\mathrm{min}} = 5\%$ gives roughly normal distribution of ϵ_{rel}.
- More difficult for ion momentum & energy sources which have $\sigma_{\mathrm{rsd}} \sim 50\%$,
  - Codes agree within error bars,
  - But, unable to detect any systematic discrepancy.
- Benchmark discussed in detail at:
  `http://w3.pppl.gov/degas2/Doc/degas2_all.pdf`

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DEGAS 2 PARALLELIZATION

- DEGAS 2 performance objectives:
  1. Should exhibit nearly linear scaling with $N_{\rm proc}$,
  2. Results independent of number & type of processors,
  3. Run over heterogeneous network of computers.
- Developed suitable random number generator,
  - Underlying arithmetic exact $\Rightarrow$ reproducible,
  - Each flight has its own random number sequence $\Rightarrow$ first step toward correlated sampling.
- PVM replaced with MPI,
  - MPI more portable and widely available,
  - Some implementations (MPICH) for heterogeneous networks.
- Load balancing needed for heterogeneous systems,
  - Break up N flights into, say, 100 "fragments",
  - "Master" passes fragments out to "slaves",
  - Faster slaves get more fragments to do.
- Must minimize communication,
  - Slaves receive problem description at start,
  - Each flight fragment contains:
    1. Index of first flight in fragment (label),
    2. Number of flights,
    3. Random number seed,
    4. Source group number.
  - At end of fragment, slave sends signal to master,
    * Master replies with another fragment,
    * Or request for results.

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- Results from each flight stored in 1 array,
  - Its data added to array for that slave's fragment,
  - Fragment data are summed into an output array.
  - To speed processing & communication, flight & fragment arrays store only nonzero elements,
    - Pointer arrays map data to full array.
  - Accuracy in accumulating data assured with:

$$M_k = M_{k-1} + (x_k - M_{k-1})/k$$
$$S_k = S_{k-1} + (x_k - M_{k-1})(x_k - M_k),$$

  - Where $M_1 = x_1$ & $S_1 = 0$,
  - $\sigma = \sqrt{S_N/(N-1)}$.
- Fig. 1: scaling of DEGAS 2 on Origin 2000 & PC cluster,
  - For 2000 flights, communication time $>$ computation time,
  - Near linear scaling for $2000N_{\rm proc}$ flights.
  - PC cluster:
    - 9 dual processor (450 MHz Pentium III) PC's,
    - Running LINUX with NAG & Portland Group compilers,
    - $2000N_{\rm proc}$ flights,
    - $\sim$ half as fast as Origin 2000 per processor.

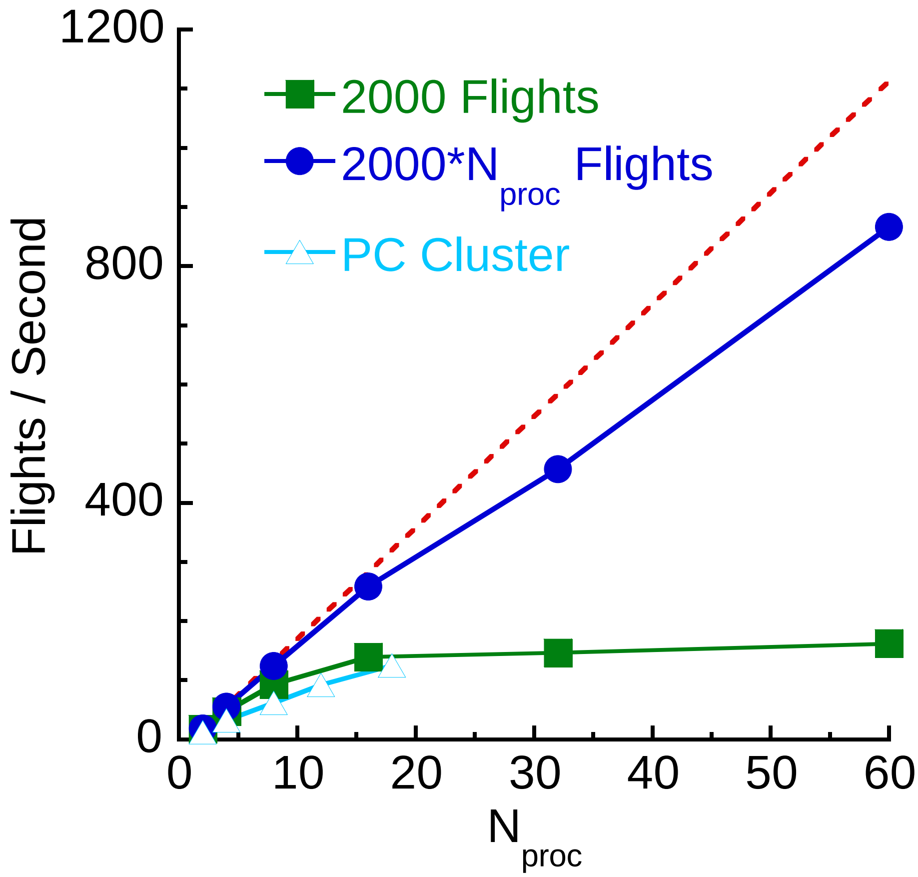

Figure 1: The processing speed of DEGAS 2 increases nearly linearly with the number of processors when the number of flights per processor is kept constant (circles for Origin 2000; triangles for a PC cluster). Ideal, linear performance for the “master - slave” paradigm is given by the dashed line. The processing rate for a constant number of flights saturates (squares).

UEDGE-DEGAS 2 COUPLING

- Coupling done same as for UEDGE-EIRENE,
  - Codes run separately,
  - Data transferred through files,
  - UEDGE run in time-dependent mode,
  - UEDGE treats DEGAS 2 sources explicitly.

- Repeat low & high power UEDGE-EIRENE runs from Rensink et al.,
  - $D = 0.5$ m^2/s,
  - $\chi_{e,i} = 0.7$ m^2/s,
  - Core plasma density $= 7 \times 10^{19}$ m^{-3},
  - Input power = 48 kW (low power) & 84 kW (high power).
- Global results match to within 7%,
- Peak temperatures differ slightly,
  - Low power: 0.9 eV for DEGAS 2, 0.8 eV for EIRENE,
  - High power: 5 eV for DEGAS 2, 6 eV for EIRENE.
  - Differences may be due to use of rescaling for particle conservation in DEGAS 2 $\Rightarrow$ effectively different recycling coefficient.
- UEDGE run times between 12 & 300 sec,
  - DEGAS 2 run on 4 Suns & ≤ 6 Dec Alphas,
  - 10,000 flights,
  - ~ 100 sec / time step outside UEDGE (high power),
  - $\sim 1/2$ spent in DEGAS 2,
  - UEDGE run time significantly shorter when DEGAS 2 uses suppressed absorption at surfaces.

COUPLING IMPROVEMENT

- Sources computed by DEGAS 2 should exactly and reproducibly reflect variations in plasma given by UEDGE,
  - Monte Carlo noise can dominate the response,
  - Correlated sampling can minimize its impact.
- Correlated sampling
  - First step: use same random number chain for a given flight,
  - Second, sample from same initial source distribution,
    - Account for source changes with weight factor,

$$w_j = S_j / S_j^0. \tag{1}$$

    - $\Rightarrow$ flight starts with same $\vec{x}$ and $\vec{v}$ in each run.
  - Tracks will eventually diverge,
  - Full correlated sampling would adjust with weights.
- Attempt to quantify effect of Eq. (1),
  - Baseline plasma from higher power UEDGE-DEGAS 2 run,
  - 1,280,000 flights, recycling source only.
  - Simulate plasma change with ad hoc perturbation in recycling source,
    - Choose so perturbation strength of 10% moves peak,
    - Conserves particles.
  - Diagnostic: ion source integrated along flux tube.
  - DEGAS 2 response: $(S_i^0 - S_i^{\text{pert}})/0.1$ $\Rightarrow$ "Reference" curve,
  - Repeat with 5000 flights at 4.5% and 5.5% perturbations $\Rightarrow$ "Standard",
  - Use Eq. (1) $\Rightarrow$ "Weighted".
  - Note difference in scale!

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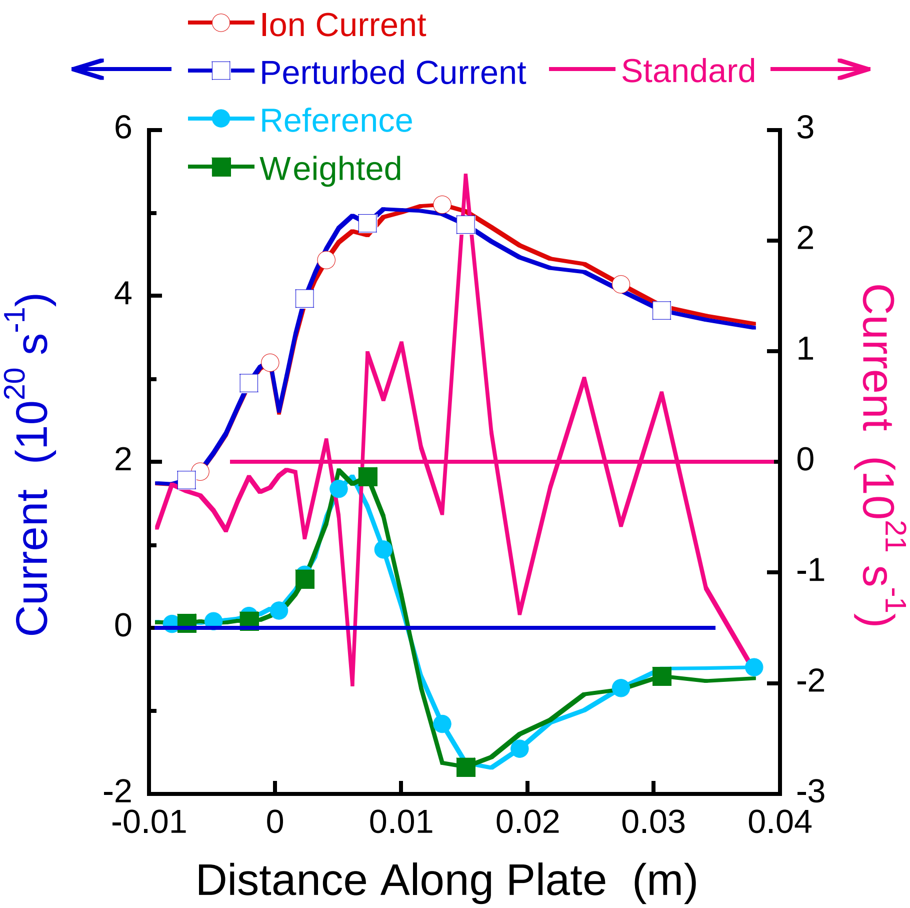

Figure 2: A 10% perturbation is added (Perturbed Current) to the ion flux to the target computed by UEDGE (Ion Current). The normalized change in the ion source integrated along a flux tube is computed with 5,000 (Standard) and 1,280,000 (Reference) flights. If the perturbation is implemented by adding weight factors, eq. 1, an accurate result (Weighted) is obtained with just 5,000 flights.

- Effect of Eq. (1) on coupled runs:
  - Fig. 3
  - Source residuals drop 30 – 40%,
  - Plasma residuals drop $\sim 20\%$.
- Doing better will require more complete correlation,
- Other options (implicit treatments) may exist.

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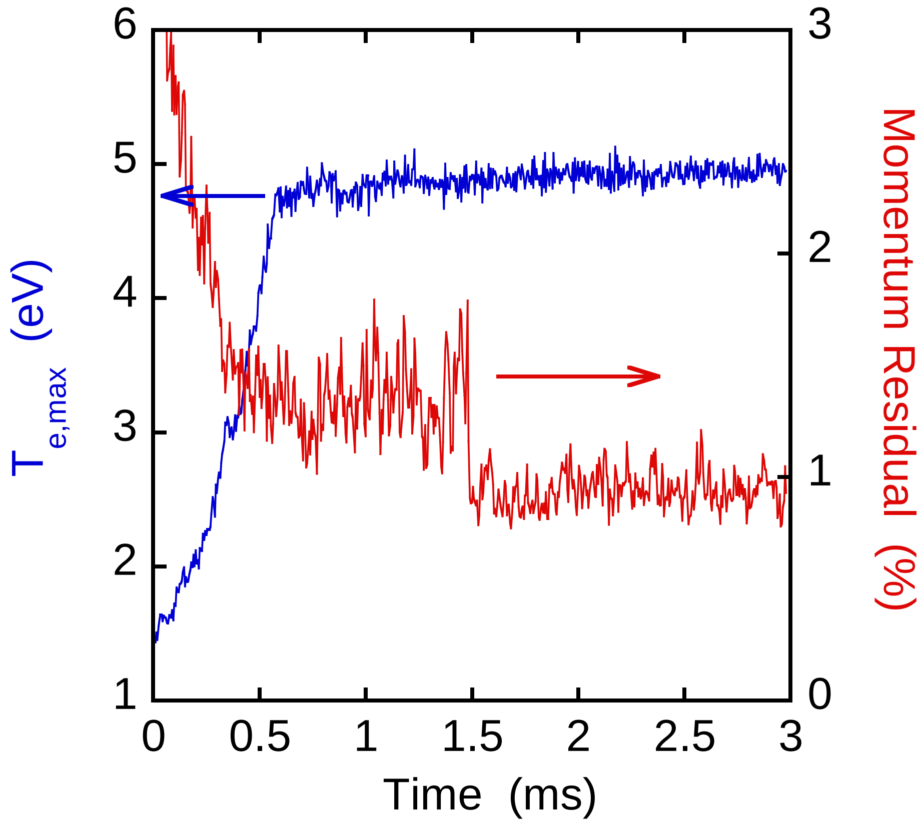


Figure 3: Time evolution of the peak electron temperature at the target in a UEDGE-DEGAS 2 run. The starting point, $t = 0$, is a self-consistent run of UEDGE with its Navier-Stokes fluid neutral model. For $t < 0.0015$, DEGAS 2 samples the source distributions directly. After $t = 0.0015$, source distribution changes are accounted for with eq. 1. The residual in the ion momentum source (gray curve) drops noticeably at this time.

EXAMPLE C-MOD RUN

- Test UEDGE-DEGAS 2 in real geometry,
- Just an example,
  - Old (1994) equilibrium,
  - UEDGE parameters from a DIII-D run,
    - n_e probably too low for C-Mod.
- Use UEDGE to generate mesh,
  - Including nonorthogonal regions to match plate shapes,
  - Add vacuum regions for DEGAS 2.
- Converges relatively quickly to steady-state,
  - Complete run required about 12 hours.

REFERENCES

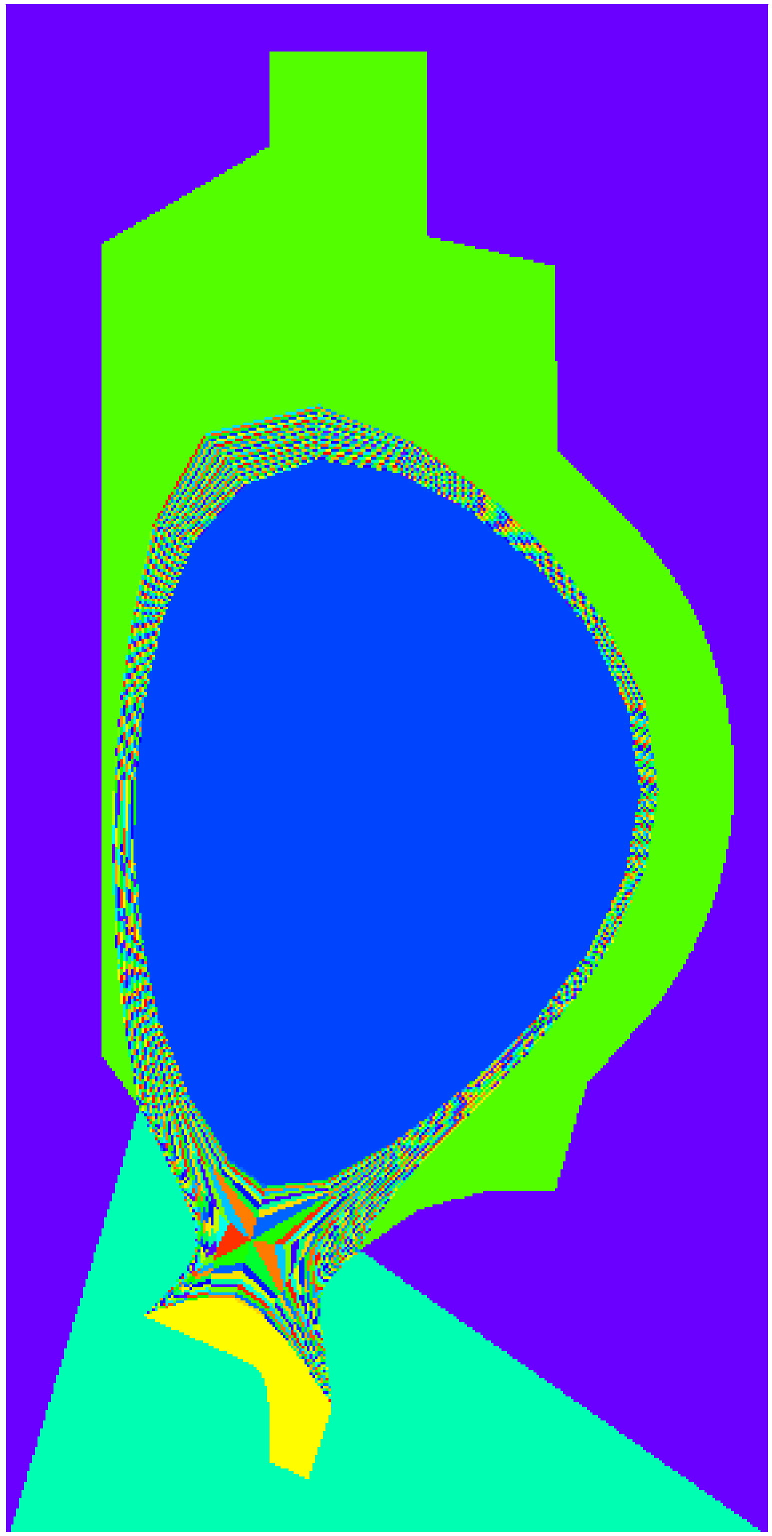
1. Stotler, D. P., Karney, C. F. F., Contrib. Plasma Phys. **34** (1994) 392
2. Rognlien, T. D. et al., Contrib. Plasma Phys. **34** (1994) 362
3. Reiter, D. et al., J. Nucl. Mater. **196–198** (1992) 80
4. Schneider, R. et al., J. Nucl. Mater. **196–198** (1992) 810
5. Rensink, M. E. et al., Contrib. Plasma Phys. **38** (1998) 325
6. Knuth, D. E., The Art of Computer Programming, Vol. 2, Addison-Wesley Publishing Company, Reading, Mass. (1981)
7. Rognlien, T. D. et al., Bull. Am. Phys. Soc. **42** (1997) 1584

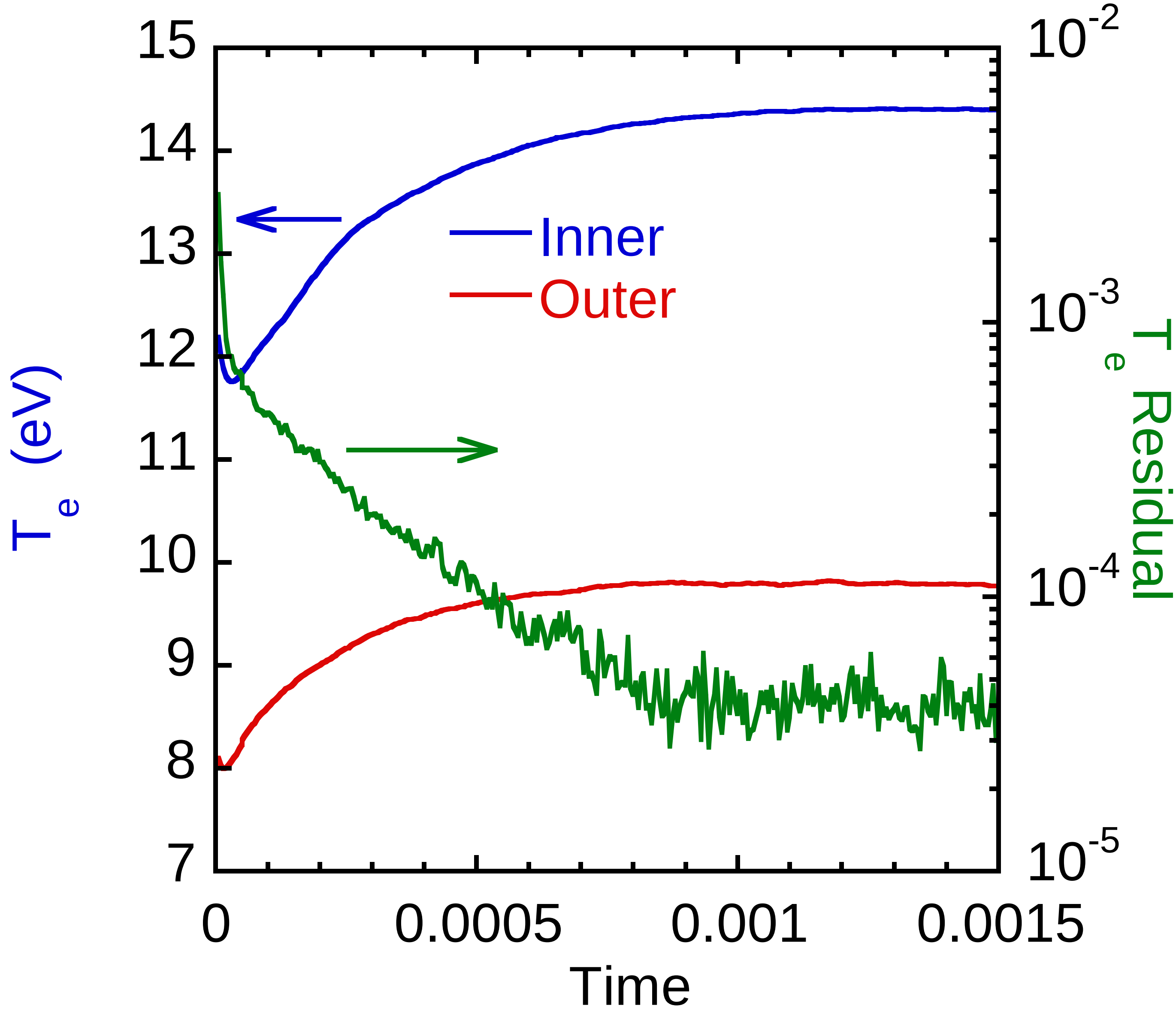
COPIES

- This poster can be found on the Web at:

  `http://w3.pppl.gov/~dstotler/pet7_poster.pdf`

- The associated paper will appear in *Contrib. Plasma Phys.* (proceedings of 7th Plasma Edge Theory Workshop)





15
14
13
12
11
10
9
8
7
0
0.0005
0.001
0.0015
Time
T e (eV)
10-2
10-3
10-4
10-5
T e Residual
Inner
Outer